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13. ABSTRACT *(Maximum 200 words)*

A brief summary of research accomplishments during the past three years is given, along with a list of publications that contain the details of this work. Also included is a list of invited presentations of ARO sponsored research. These accomplishments include: development of our Schrödinger Equation Monte Carlo (SEMC) quantum transport simulator into a powerful and efficient tool for bridging the gap from classical to quantum transport; application of our theory of "quantum capacitance" to explain experimentally observed "charging" effects in quantum dots, and to provide experimental verification of the theory; development of a method of performing electronic structure calculations via an adaptive wavelet basis; providing new insights into supposedly "old" issues including p-n junction impedance and, using SEMC, the high-order quantum effect of collision broadening; and initiation of a first principles study of hot-carrier degradation in MOS devices including the hydrogen/deuterium isotope effect.

14. SUBJECT TERMS Quantum transport, Quantum capacitance, Hot-carrier degradation, collision broadening adaptive wavelet basis.

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1 Statement of Problem Studied

The goal of our research has been the development of theoretical and numerical tools for device modeling at multiple levels, from classical to semiclassical to envelope-function quantum mechanical to atomistic quantum mechanical treatments. Important applications include the the familiar metal-oxide-semiconductor (MOS) devices and quantum well lasers.

2 Summary of Results

In the past three years we have developed our Schrödinger Equation Monte Carlo (SEMC) quantum transport simulator into a powerful and efficient tool for bridging the gap from classical to quantum transport, we have explained experimental observations of charging effects in nanostructures with our theory of quantum capacitance, we have developed a method of performing electronic structure calculations via an adaptive wavelet basis, we have begun a first principles study of hot-carrier degradation in MOS devices including the hydrogen/deuterium isotope effect, and we have provided new insights into supposedly "old" issues including p-n junction impedance and collision broadening. Important results of the first two and one-half years of this three year contract period include:

- We developed our "Schrödinger Equation Monte Carlo (SEMC)" method into a powerful, flexible, quantitatively accurate, and efficient tool for numerical simulation of transport in the realm between phase-coherent quantum transport and phase-incoherent classical transport [publications nos. 1,3,4,13]. In particular, with the addition of the ability to simulate multiple sequential scattering processes, SEMC took a major-step toward becoming a quantum analog of semiclassical Monte Carlo.

- In one application of SEMC, electron and hole capture by quantum wells was studied, a process critical to the operation of many optoelectronic devices such as quantum well lasers. The complete transition from phase-coherent to phase-incoherent transport across the well with increasing well width was exhibited — the first time such a complete transition has been exhibited via first-principles simulation — and, by comparison, the significant errors possible both with perturbative quantum approaches such as Fermi's Golden Rule, and with classical models [7].

- We substantially verified our theory of quantum capacitance [2,5] by qualitatively reproducing the experimental capacitive energy measurements of semiconductor quantum dots of S. Tarucha et al. (Phys. Rev. Lett. **77**, 3613 [1996]) [9].

- We incorporated self-consistent calculations of the dot confinement potentials into our quantum capacitance calculations to provide improved quantitative agreement to experimental data [10].

- We demonstrated experimentally that deuterium passivation was still effective after metalization steps [6].

- In initial theoretical work on the subject of hot-carrier degradation, we showed that deuterium is selected preferentially over hydrogen for surface passivation, which is important because for nominally deuterium passivated MOS devices, a significant background of hydrogen may remain [11].

- We developed a method of performing electronic structure calculations using an adaptive wavelet basis. The computational effort required should scale linearly with the number of basis functions providing significant advantages over previous methods for large atomic systems. The ultimate goal is to allow analysis of large atomic systems such as passivated silicon-oxide surfaces [12].

- We revisited the issue of p-n junction impedance, analytically resolving past misconceptions on this subject [17].

- As experts in the field of hot-carrier transport, in large part as a result of our ARO sponsored research over the years, we have provided invited articles addressing the general theory of high-field transport [14] and providing a historical perspective on the development of this theory [8], works particularly suitable for educational purposes.

A more extensive review of the work of the first approximately two and one-half years is provided by the interim progress reports. In the last seven months of the contract period we continued to build on this work:

- We wrote a comprehensive paper on the SEMC method detailing the primary features of the latest version of the code, although improvements are being made continuously [17].

- We began a study of the high-order quantum effect of collision broadening (CB) during scattering using SEMC that recently (under the new ARO contract) has lead to suggestions for fundamental yet simple changes to the treatment of CB in semiclassical Monte Carlo (SCMC) that could have profound effects on the simulation of hot-carrier effects including hot-carrier degradation [18]. In contrast to the modeling of CB in SCMC, CB is an inherent (and unavoidable) effect of allowing real scattering in SEMC.

- Scanning tunneling microscopy (STM) experiments on silicon-vacuum interfaces performed by colleagues has identified two distinct desorption mechanisms, desorption via a bonding-antibonding transition in the bond electron state, and via heating of the vibrational mode(s) of the silicon-hydrogen/bond. In our ARO sponsored research, we developed an empirical model of hot-carrier degradation in MOS devices based on the STM results, and demonstrated that both mechanisms were plausible sources of degradation in MOS devices [15,16].

- In this same work, we identified a hydrogen-deuterium isotope effect consistent with experimental results on deuterium passivated MOSFET's [15,16].

Details of the work of the past three years are provided in the referenced publications as listed in the next section.

In conclusion, we believe that this ARO sponsored research over the last three years has significantly advanced the understanding of conductance and capacitance in nano-scale devices and systems. Our work on quantum capacitance has provided a new fundamental understanding of this basic device property, much as Landauer-Büttiker theory did for conductance. SEMC now has a demonstrated ability to bridge the gap from quantum to classical transport both by allowing direct simulation of transport in systems with intermediate degrees of phase coherence, and by providing new insights into fundamental quantum processes that can be incorporated into classical and semiclassical transport studies, as in the case of modeling collision broadening in SCMC. Indeed, in this respect, our research under ARO sponsored contracts has now come full circle from the development of our full-band Monte Carlo SCMC method, to the development of our quantum transport simulator SEMC, and now back to improve SCMC. We have also begun to explore new territory with our initial steps into first-principles simulation of hot-carrier degradation, one of the most important yet, to date, poorest understood processes in semiconductor devices.

3 ARO Sponsored Publications

The following manuscripts have been published or accepted for publication during the 1995–1998 contract period:

1. Hess, P. Von Allmen, M. Grupen and L. F. Register, "Simulating Electronic Transport in Semiconductor Nanostructures," Proceedings of the *NATO Workshop on Future Trends in MIcroelectronics*, Ile de Bendor, France, July 17-21, 1995, edited by S. Luryi, J. Xu and A. Zaslavasky, (Kluer Academic Publishers, 1996) pp. 215-226.

2. G. J. Iafrate, K. Hess, J. B. Krieger, and M. Macucci, "Capacitive Nature of Atomic Size Systems," Phys. Rev. B **52**, 10737 (1995).

3. L. F. Register, "Simulation of Carrier Capture in Quantum Well Lasers Due to Strong Inelastic Scattering," Superlattices and Microstructures **18**, 223 (1995).

4. L. F. Register, "Simulation of Optical Excitation to and Emission from Electron Fabry-Perot-States Subject to Strong Inelastic Scattering, VLSI Design **6**, 351 (1998, accepted 1995).

5. M. Macucci and K. Hess, "Corrections to the Capacitance Between Two Electrodes Due to The Presence of a Quantum Confined System," VLSI Design **6**, (1998, accepted 1995).

6. I. C. Kizilyalli, J. W. Lyding and K. Hess, "Deuterium post Annealing of MOSFETs for Improved Hot Carrier Reliability," IEEE Electron Device Letters **18**, 81 (1997).

7. L. F. Register and K. Hess, "Simulation of Carrier Capture in Semiconductor Quantum Wells: Bridging the Gap from Quantum to Classical Transport," Appl. Phys. Lett. **71**, 1222 (1997).

8. K. Hess "Milestones of Hot Electron Research in Semiconductors," in *Hot Electrons in Semiconductors, Series on Semiconductor Science and Technology*, edited by N. Balkan, (Oxford University Press, 1997).

9. M. Macucci, K. Hess and G. J. Iafrate, "Numerical Simulation of Shell-filling Effects in Circular Quantum Dots," Phys. Rev. B **55**, 4879 (1997).

10. M. Macucci and K. Hess, "Shell-filling Effects in Circular Quantum dots" in Proceedings of the Fifth International Workshop on Computational Electronics, VLSI Design **8**, 443 (1998).

11. I. P. Ipatova, O. P. Chikalova-Luzian and K. Hess, "Effect of Localized Vibrations on the Si Surface Concentrations of H and D," J. Appl. Phys. **83**, 814 (1998).

12. D. A. Richie, P. Von Allmen, K. Hess and R. M. Martin, "Electronic Structure Calculations Using An Adaptive Wavelet Basis," VLSI Design **8**, 159 (1998).

13. L. F. Register, "Schrödinger Equation Monte Carlo: Bridging the Gap from Quantum to Classical Transport" in *Selected Topics in Electronics and Systems, Vol. 14: Quantum-Based Electronic Devices and Systems*, vol. ed.: M. Dutta and M. A. Stroscio, series ed.: P. K. Tien (World Scientific, Singapore, 1998) pp. 251—279, and in the International Journal of High Speed Electronics and Systems **9** 251 (1998).

14. K. Hess, "High Field Transport in Semiconductors," *Encyclopedia of Electrical Engineering* (to be published).

15. K. Hess, L. F. Register, B. Tuttle, J. Lyding and I. C. Kizilyalli, "Impact of Nanostructure Research on Conventional Solid-State Electronics: The giant Isotope effect in Hydrogen desorption and CMOS Lifetime," Physica E, to be published.

16. K. Hess, L. F. Register, B. Tuttle, J. Lyding and I. C. Kizilyalli, "Hot Carrier Degradation Issues in Submicron MOSFETSs," in *Future Trends in Microelectronics*, eds. S. Luryi, J. Xu, and A. Zaslavasky (John Wiley and Sons, New York, NY) to be published.

The following manuscripts were submitted or were in preparation during the 1995–1998 contract period, but have not yet been accepted for publication:

17. S. E. Laux and K. Hess, "New Quantitative Theory of p-n Junction Impedance: Analytical Resolution of Past Misconceptions," submitted to IEEE Transactions on Electron Devices.

18. L. F. Register and K. Hess, "Theory of Collision Broadening Through a Sequence of Scattering Events," to be submitted to Microelectronic Engineering of Elsevier.

4 Invited Presentations of ARO Sponsored Research

The following is a list of invited presentations of ARO sponsored research during the 8/95–7/98 contract period:

1. "Theoretical Study of Hydrogen and Deuterium Desorption from a Passivated SI(100) Surface," presented by P. Von Allmen at the International Conference on Quantum Devices and Circuits, Alexandria, Egypt, June 1–8, 1996.
2. "Carrier Capture in Narrow and Wide Quantum Wells: Simulation of the Transition from Weak to Strong Scattering," presented by L. F. Register at the 190th Meeting of the Electrochemical Society, San Antonio, TX, October 5–7, 1996.
3. "STM Nanofabrication and Deuterium Post Metal Annealing of MOSFETs for Improved Hot-Carrier Reliability," presented by K. Hess at the 27th IEEE Semiconductor Interface Specialists Conference, San Diego, CA, December 5–7, 1996.
4. "Electronic Transport between the Classical and Quantum Limits: Consequences of Device Speed," presented by K. Hess at the Advanced Heterostructure Workshop 1996, December 1–6, 1996, Kona, Hawaii.
5. "Dynamics of Nanostructures-STM Tunneling Current," presented by K. Hess at the Advance Heterostructure Workshop 1996, December 1–6, 1996, Kona, Hawaii.
6. "Deuterium Passivation: Device Applications," presented by K. Hess at the 24th Conference on the Physics and Chemistry of Semiconductor Interfaces, January 12–15, 1997, Research Triangle Park, NC.
7. "History of Hot Electron Degradation in MOSFETs and the Hydrogen/Deuterium Isotope effect," presented by K. Hess at the 1997 International Reliability Physics Symposium, April 7–10, 1997, Denver, C0 (tutorial).
8. "Degradation of Submicron Trough Nanoscale Silicon Devices: Implications of Recent UHV STM Measurements," presented by Karl Hess at teh Surface and Interfaces of Mesoscopic Devices conference, December 7–12, 1997, Kaanapalli, Maui, Hawaii.
9. "Impact of Nanostructure Research on Conventional Solid State Electronics," presented by K. Hess at the "New Frontiers in Low-Dimensional Physics: 10th International Winterschool on New Developments in Solid State Physics, February 23–27, 1998, Mauterndorf, Salzburg, Austria.

10. "Hot Electron Degradation Issues in Submicron CMOS," presented by K. Hess at the 1998 Advanced Research Workshop, Future Trends in Microelectronics: Off the Beaten Path, May 31–June 5, 1998, Ile des Embiez, France.

5 Scientific Personel

Scientific personnel supported in part by this project during this reporting period were:

1. Prof. Karl Hess, PI
2. Dr. Leonard F. Register, co-PI
3. Amr Haggag, M.S. student
4. David Richie, Ph.D student
5. Carl Wordelman, Ph.D. student

Prof. Hess received the the prestigious 1995 D. Sarnoff Field Award of the IEEE for his work on electronic transport in semiconductor heterolayers, he was named to the Swanlund Chair of Electrical and Computer and Computer Engineering at the University of Illinois in 1996, and he was inducted as a Fellow of the American Academy of Arts and Sciences in 1997.